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Microstructure and Cation Ordering in Sr_2AlSbO_6

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Beamline(s): X7A

Introduction: Recently the family of strontium anthimonate oxides with double perovskite structure has attracted considerable attention because of the magnetic properties presented by its members (1). Our interest in these materials is based on the great variety of symmetries found for their structures. Orthorhombic, monoclinic, tetragonal, cubic and rhomboedral space groups were suggested to describe the symmetry of different compounds of this family. In some cases even for the same compound several space groups were proposed. To the best of our knowledge this is the first report about the synthesis and structure of Sr_2AlSbO_6.

Conventional X-ray measurements revealed that the structure of this material is cubic (i.e. undistorted) double perovskite type with partially ordered Al^{3+} and Sb^{5+} cations. Cubic perovskite structures are especially suitable for the study of the ordering since in this case the superstructure reflections, i.e. those related to the B-cation ordering, are not overlapping with the order-independent reflections. The diffraction lines produced by our compound were significantly broader than those of a standard material measured on the same diffractometers. This fact suggested that the size of the crystalline grains was very small. Another interesting observation is that the superstructure reflections are even broader than the rest of the reflections.

Methods and Materials: A detector with Ge (220) analyzer crystal and a Si(111) monochromator crystal were used and the wavelength of 0.8005 Å was calibrated using a CeO_2 standard. The sample was placed in a quartz capillary and rotated during the experiment.

Results and Conclusions: Fig.1 shows a comparison between the diffraction data obtained with the different sources. A Williamson-Hall plot of the diffraction peaks in the synchrotron measurement is shown in Fig.2 (B denotes FWHM corrected for instrumental effects, θ is the diffraction angle). It can be seen that the FWHM of the superstructure reflections (triangles) are clearly bigger than those of the rest of the peaks (the superstructure reflections are relatively weak and this is the reason for the scattering of the points). Applying the Scherrer´s formula to the two sets of reflections ("normal" and superstructure) we obtained the average particle size to be about 200nm and the effective size of the ordered zones within the grains to be about 40nm. We interpret this result as an evidence that the range of ordering of the B-cations is less than the particle size. Rietveld refinement, with variable occupancy factors for the Al y Sb atoms, of the synchrotron diffraction data showed that about 80% of the B-cations occupy their respective sites.

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References:

1. E.J. Cussen, J.F. Vente, P.D. Battle, T.C. Gibb, J. Mater. Chem, **7** (3), 1997, 459-463

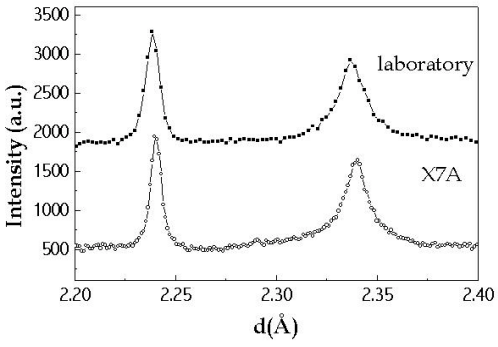

Figure 1. Comparison between the diffraction data obtained with the different sources.

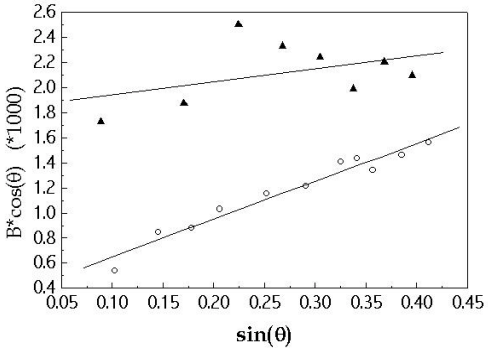

Figure 2. Williamson-Hall plot of the diffraction peaks from the synchrotron measurements.